Journal of Low Temperature Physics 2016, pages 1-6

Analysis of Electronic and Structural Properties of Surfaces and Interfaces Based on LaAlO3 and SrTiO3

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Abstract

© 2016 Springer Science+Business Media New York Recently, it was established that a two-dimensional electron system can arise at the interface between two oxide insulators LaAlO(Formula presented.) and SrTiO(Formula presented.). This paradigmatic example exhibits metallic behaviors and magnetic properties between non-magnetic and insulating oxides. Despite a huge amount of theoretical and experimental work a thorough understanding is yet to be achieved. We analyzed the structural deformations of a LaAlO(Formula presented.) (001) slab induced by hydrogen adatoms and oxygen vacancies at its surface by means of density functional theory. Moreover, we investigated the influence of surface reconstruction on the density of states and determined the change of the local density of states at the Fermi level with increasing distance from the surface for bare LaAlO(Formula presented.) and for a conducting LaAlO(Formula presented.)/SrTiO(Formula presented.) interface. In addition, the Al-atom displacements and distortions of the TiO(Formula presented.)-octahedra were estimated.

http://dx.doi.org/10.1007/s10909-016-1483-2

Keywords

Defects, Density functional, Electronic structure, Interface, LAO/STO, Surface